International Journal of Quantum Chemistry
Author Index—Volume 71

Aiga, F.
—; Tada, T.: Multiple Cluster Model (MCM) for Surface Reaction Systems, 403
See Shiga, M., 251
Alikhani, M. E.
Structural, Vibrational, and Bonding Analysis of M_2—SiO (M = Li or Ag) Using Density Functional Theory, 499
Almeida, A. L.
—; Martins, J. B. L.; Taft, C. A.; Longo, E.; Lester, Jr., W. A.,: Theoretical Study of Water Coverage on MgO Surfaces, 153
Angeles, E. See Cogordan, J. A., 415
Angulo, J. C.
—; Romera, E.: Improved Upper Bounds for the Atomic Ionization Potential, 185
Arias de Saavedra, F. See Porras, I., 443

Cadilhe, M. W.
—; Soares Neto, J. J.: Classical Four-Body Problem in Hyperspherical Coordinates, 15
Cheng, Y. See Maofa, G., 313
Chiachung, S. See Maofa, G., 313
Cogordan, J. A.
—; Mayoral, M.; Angeles, E.; Toscano, R. A.; Martínez, R.: Neuroleptic and Antidepressant Tricyclic Compounds: Theoretical Study for Predicting Their Biological Activity by Semiempirical, Density Functional, and Hartree–Fock Methods, 415
Cundari, T. R.
—; Fu, W.: Reaction Pathways for Model II–VI Precursors: A Computational Study, 47

Dai, Y.
—; Ding, S.-L.: Lie Algebraic Approach to Multiphoton Excitation of Diatomic Molecules in Intense Laser Fields, 201
Davidov, G.
—; Fuks, D.; Dorfman, S.; Krasko, G. L.: Volume-Dependent Potential Approach for Tungsten, 343
Defranceschi, M.
—; Le Bris, C.: Computing a Molecule in Its Environment: A Mathematical Viewpoint, 227
Deumans, E.
Review of *Path Integral Methods*, T. Kashiwa, Y. Ohnuki, and M. Suzuki, 513
Ding, S.-L. See Dai, Y., 201
Dorfman, S. See Davidov, G., 343
Dunne, L. J.
—; Application of the Field-Theoretic Method of Bohm and Pines to a Study of the Metal–Insulator Transition in Doped Dielectric Media, 111

Eid, R.
Higher Order Finite Element Solution of the One-Dimensional Schrödinger Equation, 147
El-Taher, S.
Theoretical Study on the Gas-Phase Reactivity of Halogenated Alkylperoxyl Radicals Toward Alkenes, 273

Feldmann, D. M. See Porras, I., 455
Fu, W. See Cundari, T. R., 47
Fuks, D. See Davidov, G., 343

Gaftoi, V. See Morales, J., 465
Gardiner, W. C. See Monaco, R. R., 57
Gómez-Jeria, J. S.
—; Lagos-Arancibia, L.: Quantum-Chemical Structure-Affinity Studies on Kynurenic Acid Derivatives as Gly/NMDA Receptor Ligands, 505
Gurin, V. S.
Quantum Chemistry of Quantum Size-Effects in Semiconductors: Small Clusters Electronic Structure Calculations, 337

Haas, Y. See Zilberg, S., 133
Harland, P. W. See Hu, W.-P., 75
Harris, S. A. See Hu, W.-P., 75
Hu, W.-P.
—; Harris, S. A.; Harland, P. W.; Phillips, L. F.: Collisional Reorientation of Symmetric-Top Molecules in Stark Fields, 75

Ichikawa, H.
—; Yoshida, A.: Complete One- and Two-Center Partitioning Scheme for the Total Energy in the Hartree–Fock Theory, 35
Ikegami, H.
Coherent Positronium Molecules Ps_n and Scanning Clustering Microscopy, 83

Jikang, F. See Maofa, G., 313
Jorge, F. E.
—; Muniz, E. P.: Accurate Adapted Gaussian Basis Sets for the Atoms from H Through Xe, 307
Judge, R. H. See Moule, D. C., 167
Jursic, B. S.
High-Level Ab Initio Computational Study of Doublet and Quartet Nitrogen Reaction with Methane, 481

Kanayama, K. See Koga, T., 491
Karelson, M. See Tamm, T., 101

Kennedy, H. L.
—; Zhao, Y.: Evaluation of Integrals over STOs on Different Centers and the Complementary Convergence Characteristics of Ellipsoidal-Coordinate and Zeta-Function Expansions, 1
King, F. W. See Porras, I., 455
Kirschner, S. See Monaco, R. R., 57
Koga, T.
—; Kanayama, K.; Watanabe, S.; Thakkar, A. J.: Analytical Hartree–Fock Wave Functions Subject of Cusp and Asymptotic Constraints: He to Xe, Li^+ to Cs^+, H^- to I^-, 491
Komninos, Y.
—; Nicolaides, C. A.: Molecular Shape, Shape of the Geometrically Active Atomic States, and Hybridization, 25
Krasko, G. L. See Davidov, G., 343
Kubli-Garfias, C.
Comparative Study of the Electronic Structure of Pregnanolones by Ab Initio theory, 433
Kumar, A. See Mishra, P. C., 191

Ladik, J. See Wechsler, D., 285
Lagos-Arancibia, L. See Gómez-Jeria, J. S., 505
Le Bris, C. See Defranceschi, M., 227
Lester, Jr., W. A. See Almeida, A. L., 153
Lichanot, A. See Mérawa, M., 63
Lim, E. C. See Moule, D. C., 167
Liu, H. See Moule, D. C., 167
Longo, E. See Almeida, A. L., 153
Lukovits, I.
—; Nikolić, S.; Trinajstić, N.: Resistance Distance in Regular Graphs, 217

Maofa, G.
—; Jikang, F.; Cheng, Y.; Zhiru, L.; Chiachung, S.: Ab Initio DFT Studies on Ti_nC_{2n} (n = 1–6) Clusters, 313
Martínez, R. See Cogordan, J. A., 415
Martins, J. B. L. See Almeida, A. L., 153
Mayoral, M. See Cogordan, J. A., 415
Mérawa, M.
—; Rérat, M.; Lichanot, A.: Compton Profiles and Polarizability as Two Similar Probes of the Electronic Structure of 14 Electron Diatomic Molecules: An Ab Initio Study, 63
Mishra, P. C.
—; Kumar, A.: Modified Hybridization Displacement Charge Scheme for π-Electron Systems: Study of Molecular Electrostatic Potential Maps, 191
Monaco, R. R.
—; Gardiner, W. C.; Kirschner, S.: Semiempirical Studies of Ring Twisting in *cis*-Stilbene and Related Biomolecules, 57
Monkhorst, H. J.
Review of *Coulomb Interactions in Nuclear and Atomic Few-Body Collisions*, by Frank S. Levin and David A. Micha, Eds.
Morales, J.
—; Peña, J. J.; Ovando, G.; Gaftoi, V.: Generalized Potentials: Free Particle, Harmonic, and Morse Partner Potentials, 465
Mosyagin, N. S. See Titov, A. V., 359
Moule, D. C.
—; Judge, R. H.; Liu, H.; Lim, E. C.: Torsional Symmetry Dependence of S_1 Dynamics in Molecules that Undergo Methyl Internal Rotation, 167
Moyano, G. E.
—; Villaveces, J. L.: Approximation to Wave Functions, Energies, and Energy Derivatives for Molecular Systems Based on Distribution Theory, 121
Muniz, E. P. See Jorge, F. E., 307

Nagao, H. See Nakano, M., 295
See Yamada, S., 177
Nakano, M.
—; Yamada, S.; Nagao, H.; Yamaguchi, K.: Numerical Coupled Liouville Approach: Application to Second Hyperpolarizability of Molecular Aggregate, 295
See Yamada, S., 177
See Yamada, S., 329
Nicolaides, C. A.
On the Application of Conventional Quantum Chemistry Methods of Computation to States Perturbed by the Continuous Spectrum, 209
See Komninos, Y., 25
Nikolić, S. See Lukovits, I., 217

Oliva, J. M.
Bonding in Benzene Methylene Isomers: Modern VB Study Using Spin-Coupled Theory, 319
Ovando, G. See Morales, J., 465

Patra, S. M.
—; Vishveshwara, S.: Classification of Polymer Structures by Graph Theory, 349
Peña, J. J. See Morales, J., 465
Phillips, L. F. See Hu, W.-P., 75
Porras, I.
—; Arias de Saavedra, F.: Description of Correlated Densities for Few-Electron Atoms by Simple Functional Forms, 443
—; Feldmann, D. M.; King, F. W.: A Nonlinear Programming Approach to Lower Bounds for the Ground-State Energy of Helium, 455

Rérat, M. See Mérawa, M., 63
Romera, E. See Angulo, J. C., 185

Sabin, J.
Review of *Fuzzy Logic in Chemistry*, D. H. Rouvray, Ed., 441
Sahni, V.
—; Slamet, M.: Electron Correlations in Kohn–Sham Exchange-Only Theory, 473
Sasagane, K. See Shiga, M., 251
Shiga, M.
—; Aiga, F.; Sasagane, K.: Dynamic Hyperpolarizabilities in Møller–Plesset Perturbation Theory, 251

Slamet, M. See Sahni, V., 473
Soares Neto, J. J. See Cadilhe, M. W., 15

Tada, T. See Aiga, F., 403
Taft, C. A. See Almeida, A. L., 153
Tamm, J. See Tamm, T., 101
Tamm, T.
—; Tamm, J.; Karelson, M.: A Quantum-Mechanical Study of Oxidized Oligopyrroles, 101
Thakkar, A. J. See Koga, T., 491
Titov, A. V.
—; Mosyagin, N. S.: Generalized Relativistic Effective Core Potential: Theoretical Grounds, 359
Toscano, R. A. See Cogordan, J. A., 415
Trinajstić, N. See Lukovits, I., 217

Villaveces, J. L. See Moyano, G. E., 121
Vishveshwara, S. See Patra, S. M., 349

Watanabe, S. See Koga, T., 491
Wechsler, D.
—; Ladik, J.: Contribution to the Theory of High-Temperature Superconductivity in $YBa_2CU_3O_7$, 285

Yamada, S.
—; Nakano, M.; Nagao, H.; Yamaguchi, K.: Electron Correlation and Structure Dependencies of the Second Hyperpolarizability of Ethylene, 177
—; Nakano, M.; Yamaguchi, K.: CAS–SCF and Density Functional Calculations of Second Hyperpolarizabilities for a Nitronyl Nitroxide Radical, 329
See Nakano, M., 295
Yamaguchi, K. See Nakano, M., 295
See Yamada, S., 177
See Yamada, S., 329
Yoshida, A. See Ichikawa, H., 35

Zerner, M. C.
Review of *Mathematics for Chemistry*, by Graham Doggett, 215
Zhao, Y. See Kennedy, H. L., 1
Zhiru, L. See Maofa, G., 313
Zilberg, S.
—; Haas, Y.: The Electron-Pair Origin of Antiaromaticity: Spectroscopic Manifestations, 133

International Journal of Quantum Chemistry Subject Index—Volume 71

Ab initio, 153
Ab initio calculations, 63, 337, 433, 481
Ab initio density functional theory (DFT), 313
Activation enthalpy, 273
Adapted Gaussian basis set, 307
Adduct formation, 47
Adsorption, 153
AM1, 57
AM1 and PM3, 273
Antiaromaticity, 133
Asymptotic behavior, 491
Atomic density functionals, 185
Atomic hybridization dipole moment, 191
Atomic ionization potential, 185
Atomic structure, 443
Atoms, 491

Band structure calculations, 343
Beam-defocusing collisions, 75
Benzene methylene isomers, 319
BF CO N_2, 63
Biological activity prediction, 415
Bohm–Pines method, 111
Bond index, 35
Born–Oppenheimer approximation, 121
B3LYP density functional, 209

Catalytic activity, 83
Chain length, 101
Clusters, 337
Coherent annihilation, 83
Coherent positronium molecule, 83
Collisional reorientation, 75
Combretastatin, 57
Complete active space self-consistent-field (CAS–SCF) calculations, 329
Compton profiles, 63
Conjugated cyclic hydrocarbons, 133
Convergence, 1
Coupled Liouville equations, 295
Cusp condition, 491
Cusp-conditions, 443
Cyclic clusters, 313

Density functional (DF) methods, 329
Density functional theory, 499
Density matrix, 403
Density-of-states moments, 343
Distribution theory, 121
Doped dielectric, 111
Doped polypyrrole, 101
Dynamic hyperpolarizabilities, 251

Eigenvalues, 349
Eigenvectors, 349
Electromagnetic fields, 227
Electron affinities, 209
Electron correlation, 177
Electron correlations, 473
Electron density, 185, 443
Electron pairs, 133
Electronic structure, 63, 433
Energy partitioning scheme, 35
Epipregnanolone, 433
Ethylene, 177
Exchange–correlation functionals, 329

Finite element, 147
5β-progestins, 433
Four-body problem, 15
Friedel oscillations, 111
Frozen-core approximation, 359

Gas-phase reactivity, 273
Gaussian approximation, 359
Generalized functions, 121
Generalized potentials, 465
Generalized relativistic effective core potential (GRECP), 359
Generator coordinate Hartree–Fock method, 307
Geometrically active atomic state, 25
Geometry optimization, 403
Gly/NMDA site, 505
Graph invariant, 217
Graph theory, 349

Hamiltonian, 359, 465
Hartree–Fock, 185, 491
Hartree–Fock theory, 35
Helium, 455
High-temperature superconductivity, 285
Hunbury Brown–Twiss effect, 83
Hybridization, 25
Hybridization displacement charge scheme (HDC-PI), 191
Hyperspherical coordinates, 15

Integrals, 1
Isolated molecular system, 227
Isospectral Hamiltonian, 465

Kohn–Sham exchange-only theory, 473
Kynurenic acid derivatives, 505

Laser, 201
Lattice model, 349
Lie algebra, 201
Linear combination of atomic orbitals, 403
Long-range collisions, 75
Lower bounds, 455
Lowest excited singlet state (S_1), 167

Maximum spin states, 25
Met-Cars, 313
Metal–nonmetal transition, 111
Methane, 481
Methyl internal rotation, 167
MgO, 153
MNDO, 57
Model II–VI precursors, 47
Molecular aggregates, 295
Molecular electrostatic potential (MEP) features, 191
Molecular orbital calculation, 251
Molecular shape, 25

Møller–Plesset perturbation theory, 251
M_2—SiO (M = Li or Ag) complexes, 499
Multiphoton, 201
Multiple cluster model, 403

Nonbonded interaction, 349
Nonlinear programming, 455

Oligomers, 101
Oligopyrroles, 101
OMVPE of II–VI materials, 47
One-dimensional Schrödinger equation, 147
Optimized potential method (OPM), 473

Partner potentials, 465
Pauling's bond strength function, 25
Peroxyl radicals, 273
π-electrons, 191
π-bonds, 319
Plasma modes, 111
Polarizability, 63
Polymer conformation, 349
Potential-energy surface, 481
Potential energy surfaces, 121
Pregnanedione, 433
Pregnanolone, 433
Progesterone, 433

QCIDS(T), 209
Quantum-chemical structure–affinity relationship, 505
Quartet nitrogen, 481
Quasienergy derivatives method, 251

Radical addition, 273
Reaction dynamics, 15
Resistance distance, 217
Rotation coupling, 167

Sadlej basis set, 251
SAM1, 57
Scaling of wave function, 35
Scanning clustering microscopy, 83
Second hyperpolarizability, 295
Second hyperpolarizability (γ), 177
Selection rules for collisions, 75
Semiconductors, 337
Semiempirical quantum mechanical models, 57
Slater-type functions, 491
Slater-type orbitals, 1
Specific potentials, 465
Spin-coupled theory, 319
Stark states, 75
Stilbene, 57
Structure dependencies, 177
Subatomic scale scanning, 83
Superconductivity, 285
Surface, 153, 403

Testing functions space, 121
Theoretical methods, 415
Thermal properties, 343
Torsional symmetry, 167
Total energy results, 307
Tricyclic psychotropic agents, 415
Truncated domain, 147
Tungsten, 343
Two-electron and three-electron atoms, 443

Upper bounds, 185

Vibration-rotation, 201

Water coverage, 153

$YBa_2Cu_3O_7$, 285